

Pentachloroethane
76-01-7 | DTXSID7021104

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -18.3 °C

Global applicability domain: Inside

Local applicability domain index: 6.32e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

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Pentachloroethane

Measured: -29.0

Predicted: -18.3

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Bromotrichloromethane

Measured: -5.70

Predicted: -21.9

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Propane, 1,1,1,3,3,3-hexachloro-

Measured: -27.0

Predicted: 6.11e-01

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Propane, 1,1,1,2,3,3,3-heptachloro-

Measured: 11.0

Predicted: 11.8